

# Average Mixing of Continuous Quantum Walks

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## Abstract

If  $X$  is a graph with adjacency matrix  $A$ , then we define  $H(t)$  to be the operator  $\exp(itA)$ . The Schur (or entrywise) product  $H(t) \circ H(-t)$  is a doubly stochastic matrix and because of work related to quantum computing, we are concerned with the *average mixing matrix*  $\widehat{M}_X$ , defined by

$$\widehat{M}_X = \lim_{C \rightarrow \infty} \frac{1}{C} \int_0^C H(t) \circ H(-t) dt.$$

In this paper we establish some of the basic properties of this matrix, showing that it is positive semidefinite and that its entries are always rational. We see that in a number of cases its form is surprisingly simple. Thus for the path on  $n$  vertices it is equal to

$$\frac{1}{2n+2}(2J + I + T)$$

where  $T$  is the permutation matrix that swaps  $j$  and  $n+1-j$  for each  $j$ . If  $X$  is an odd cycle or, more generally, if  $X$  is one of the graphs in a pseudocyclic association scheme on  $n$  vertices with  $d$  classes, each of valency  $m$ , then its average mixing matrix is

$$\frac{n-m+1}{n^2}J + \frac{m-1}{n}I.$$

(One reason this is interesting is that a graph in a pseudocyclic scheme may have trivial automorphism group, and then the mixing matrix is more symmetric than the graph itself.)

# 1 Average Mixing

Let  $X$  be a graph with adjacency matrix  $A$ . We define a transition matrix  $H_X(t)$  by

$$H_X(t) := \exp(itA).$$

For a physicist this matrix determines a continuous quantum walk. We note that it is both symmetric and unitary, in particular  $\overline{H_X(t)} = H_X(-t)$ . For relevant recent surveys see, e.g., Kendon and Tamon [6], Godsil [4].

The matrix  $H(t)$  gives rise to a family of probability densities as follows. Let  $A \circ B$  denote the *Schur product* of two matrices  $A$  and  $B$  with the same order. Thus

$$(A \circ B)_{u,v} = A_{u,v} B_{u,v}.$$

and we will use  $A^{\circ 2}$  to denote  $A \circ A$ . Then if

$$M_X(t) := H_X(t) \circ H_X(-t)$$

we see that  $M_X(t)$  is a nonnegative real matrix and, since  $H_X(t)$  is unitary, each row and column of  $M_X(t)$  sums to 1. We use  $e_u$  to denote the standard basis vector of  $\mathbb{C}^{V(X)}$  indexed by the vertex  $u$ , thus we have a family of probability densities  $e_u^T M_X(t)$ , and we are concerned with the behavior of these densities. In this paper we are interested in the matrix  $\widehat{M}_X$ , which we define by

$$\widehat{M}_X = \frac{1}{C} \int_0^C M_X(t) dt.$$

Following [1], we call this the *average mixing matrix* of  $X$ .

To work with  $M_X$  and  $\widehat{M}_X$ , we use the spectral decomposition of  $A$ . This allows us to write  $A$  as

$$A = \sum_r \theta_r E_r$$

where  $\theta_r$  runs over the distinct eigenvalues of  $A$  and  $E_r$  is the matrix representing orthogonal projection onto the eigenspace belonging to  $\theta_r$ . Then we have

$$H_X(t) = \sum_r \exp(i\theta_r t) E_r$$

and

$$M_X(t) = \sum_r E_r^{\circ 2} + 2 \sum_{r < s} \cos((\theta_r - \theta_s)t) E_r \circ E_s.$$

From this we have:

**1.1 Lemma.** If  $A = \sum_r \theta_r E_r$  is the spectral decomposition of  $S = A(X)$ , then

$$\widehat{M}_X = \sum_r E_r^{\circ 2}. \quad \square$$

## 2 Properties of the Average Mixing Matrix

In this section we derive some basis properties of the average mixing matrix. We know already that it is symmetric. By a famous theorem of Schur, the Schur product  $M \circ N$  of two positive semidefinite matrices is positive semidefinite and, since the sum of positive semidefinite matrices is positive semidefinite, we see that  $\widehat{M}_X$  is positive semidefinite. If  $A$  and  $B$  are symmetric matrices of the same order, we write  $A \succcurlyeq B$  to denote that  $A - B$  is positive semidefinite.

Clearly  $\widehat{M}_X$  is a nonnegative matrix. In fact:

**2.1 Lemma.** If  $X$  is connected, all entries of  $\widehat{M}_X$  are positive.

*Proof.* Each Schur square  $E_r^{\circ 2}$  is nonnegative and if  $(\widehat{M}_X)_{u,v} = 0$  then  $(E_r^{\circ 2})_{u,v} = 0$ . However this implies that  $(E_r)_{u,v} = 0$  for all  $r$  and hence any linear combination of the idempotents  $E_r$  has  $uv$ -entry zero. Since this implies that  $(A^k)_{u,v} = 0$  for all  $k$  we conclude that  $X$  is not connected.  $\square$

In [4, Lemma 16.2] we show that average mixing is never uniform, that is,  $\widehat{M}_X$  cannot be a scalar multiple of the all-ones matrix  $J$ .

We say that a matrix  $M$  is a *contraction* if  $x^* M x \leq x^* x$  for all complex vectors  $x$ .

**2.2 Lemma.** If  $\widehat{M}_X$  is the average mixing matrix of the graph  $X$  then all eigenvalues of  $\widehat{M}_X$  lie in the interval  $[0, 1]$ .

*Proof.* Since  $H(t) \otimes H(-t)$  is unitary and since  $H(t) \circ H(-t)$  is a principal submatrix of  $H(t) \otimes H(-t)$ , it follows that  $H(t) \circ H(-t)$  is a contraction. Since it is symmetric and real, its eigenvalues must lie in the interval  $[0, 1]$ , and therefore this holds true for  $\widehat{M}_X$  too.  $\square$

Since  $\widehat{M}_X$  is the average of doubly stochastic matrices, it is doubly stochastic and its largest eigenvalue is 1. We can also see this without appealing to the averaging. Notice that

$$((E_r \circ E_r)\mathbf{1})_u = ((e_u^T E_r) \circ (e_u^T E_r))\mathbf{1} = \langle e_u^T E_r, e_u^T E_r \rangle = e_u^T E_r^2 e_u = e_u^T E_r e_u = (E_r)_{u,u}$$

and, since  $\sum_r E_r = I$ , it follows that  $\widehat{M}_X \mathbf{1} = \mathbf{1}$ .

**2.3 Lemma.** *The average mixing matrix of a graph is rational.*

*Proof.* Let  $\phi(X, x)$  be the characteristic polynomial of  $X$ , and let  $\mathbb{F}$  be a splitting field for  $\phi(X, x)$ . We use the fact that an element of  $\mathbb{F}$  which is fixed by all field automorphisms of  $\mathbb{F}$  must be rational. If  $\sigma$  is an automorphism of  $\mathbb{F}$ , then

$$A = A^\sigma = \sum_r \theta_r^\sigma E_r^\sigma.$$

Since  $\theta_r^\sigma$  must be an eigenvalue of  $A$  and since the spectral decomposition of  $A$  is unique, it follows that  $E_r^\sigma$  is one of the idempotents in the spectral decomposition of  $A$ . Therefore the set of idempotents is closed under field automorphisms, and so must the  $\{E_r^{\sigma^2}\}_r$ . Consequently

$$\widehat{M}_X^\sigma = \widehat{M}_X$$

for all  $\sigma$  and therefore  $\widehat{M}_X$  is rational.  $\square$

Note that this lemma holds whether we use the Laplacian or the adjacency matrix—all we need is that  $A$  be symmetric with integer entries.

We use  $L(X)$  to denote the Laplacian matrix  $X$ . If  $\Delta$  is the diagonal matrix whose  $i$ -th diagonal entry is the valency of the  $i$ -vertex of  $X$ , then

$$L(X) = \Delta - A.$$

The transition matrix of  $X$  relative to  $L(X)$  is

$$H_L(t) := \exp(it(\Delta - A)).$$

When  $X$  is regular, questions about  $H_L$  reduce immediately to questions about  $H_X$ , but in general there is no simple relation between the two cases.

**2.4 Lemma.** *If  $X$  is regular then  $X$  and its complement  $\overline{X}$  have the same average mixing matrix. For any graph  $X$ , the average mixing matrix relative to the Laplacian of  $X$  is equal to the average mixing matrix relative to the Laplacian of  $\overline{X}$ .*

*Proof.* If  $X$  is regular then the idempotents in the spectral decomposition of its adjacency matrix are the idempotents in the spectral decomposition of the adjacency matrix of  $\overline{X}$ . For any graph  $X$  on  $n$  vertices

$$L(\overline{X}) = L(K_n) - L(X);$$

since  $L(K_n) = nI - J$  and since  $L(X)$  commutes with  $J$ , the idempotents in the spectral decomposition of its Laplacian are the idempotents in the spectral decomposition of the Laplacian of  $\overline{X}$ .  $\square$

### 3 Integrality

In investigating the relation between the structure of  $\widehat{M}_X$  and the graph  $X$ , it can be convenient to scale  $\widehat{M}_X$  so that its entries are integers. For this we need to know a common multiple of the denominators of its entries.

**3.1 Lemma.** *If  $D$  is the discriminant of the minimal polynomial of  $A$ , then  $D^2 \widehat{M}_X$  is an integer matrix.*

*Proof.* Let  $\theta_1, \dots, \theta_m$  be the distinct eigenvalues of  $A$ . Define polynomials  $\ell_r(t)$  by

$$\ell_r(t) := \prod_{s \neq r} (t - \theta_s).$$

We note that  $\ell_r(\theta_r) = \psi'(\theta_r)$  and

$$\frac{\ell_r(\theta_s)}{\psi'(\theta_r)} = \delta_{r,s}.$$

Now

$$E_r = \frac{1}{\psi'(\theta_r)} \ell_r(A).$$

The discriminant  $D$  of  $\psi$  is equal (up to sign) to

$$\prod_{r=1}^m \psi'(\theta_r);$$

since the entries of  $\ell_r(A)$  are algebraic integers we conclude that the entries of  $D^2 E_r$  are algebraic integers and therefore the entries of  $D^2 \widehat{M}_X$  are algebraic integers. Since  $\widehat{M}_X$  is rational, the lemma follows.  $\square$

We have no reason to believe this lemma is optimal. If the eigenvalues of  $X$  are all simple, we can do better.

**3.2 Theorem.** *Let  $X$  be a graph with all eigenvalues simple and let  $D$  be the discriminant of its characteristic polynomial. Then  $D \widehat{M}_X$  is an integer matrix.*

*Proof.* We have

$$(xI - A)^{-1} = \sum_r \frac{1}{x - \theta_r} E_r$$

and since  $(I - tA)^{-1}$  is the walk generating function of  $X$ , it follows from [3, Corollary 4.1.3] that

$$(E_r)_{u,v} = \lim_{x \rightarrow \theta_r} \frac{(x - \theta_r) (\phi(X \setminus u, x) \phi(X \setminus v, x) - \phi(X \setminus uv, x) \phi(X, x))^{1/2}}{\phi(X, x)}$$

and since

$$\lim_{x \rightarrow \theta_r} \frac{\phi(X, x)}{x - \theta_r} = \phi'(X, \theta_r)$$

we conclude that if  $\theta_r$  is simple

$$((E_r)_{u,v})^2 = \frac{\phi(X \setminus u, \theta_r) \phi(X \setminus v, \theta_r)}{\phi'(X, \theta_r)^2}.$$

If  $B$  is the  $n \times n$  matrix with  $ur$ -entry  $\phi(X \setminus u, \theta_r)$  and  $\Delta$  is the  $n \times n$  diagonal matrix with  $r$ -th diagonal entry  $\phi'(X, \theta_r)$ , it follows that

$$\widehat{M}_X = B \Delta^{-2} B^T.$$

Assume  $n = |V(X)|$  and let  $\theta_1, \dots, \theta_n$  be the eigenvalues of  $X$ . Let  $V$  be the  $n \times n$  Vandermonde matrix with  $ij$ -entry  $\theta_j^{i-1}$ . Let  $\phi$  be the characteristic polynomial of  $X$ . The discriminant of  $\phi$  is equal to the product of the entries of  $\Delta$ , we denote it by  $D$ .

Let  $C$  be the  $n \times n$  matrix whose  $ur$ -entry is the coefficient of  $x^{r-1}$  in  $\phi(X \setminus u, x)$ . Then  $CV = B$  and

$$\widehat{M}_X = CV \Delta^{-2} V^T C^T.$$

Define polynomials  $\ell_s(x)$  by

$$\ell_s(x) = \prod_{r \neq s} (x - \theta_r)$$

and let  $L$  be the  $n \times n$  matrix with  $sj$ -entry equal to the coefficient of  $x^{j-1}$  in  $\ell_s(x)$ . Note that

$$\ell_s(\theta_r) = \delta_{r,s} \phi'(\theta_s)$$

and therefore

$$LV = \Delta.$$

Since

$$\Delta = \Delta^T = V^T L^T$$

it follows that

$$\Delta^{-2} = V^{-1} L^{-1} L^{-T} V^{-T}$$

and so

$$V \Delta^{-2} V^T = V V^{-1} L^{-1} L^{-T} V^{-T} V^T = (L^T L)^{-1}.$$

(We're almost done.) The entries of  $L$  are algebraic integers. As

$$\det(VV^T) = \det(V)^2 = D$$

and as  $LD = \Delta$ , we see that  $\det(L^T L) = D$ . Therefore the entries of

$$D(L^T L)^{-1}$$

are algebraic integers. So the entries of  $DV\Delta^{-2}V^T$  are algebraic integers and, since the entries of  $C$  are integers, the entries of  $D\widehat{M}_X$  are algebraic integers. But the entries of  $D\widehat{M}_X$  are rational and therefore they are all integers.  $\square$

It is at least plausible that if  $D$  is the discriminant of the minimal polynomial of  $X$ , then  $D\widehat{M}_X$  is an integer matrix.

## 4 Average Mixing on Paths

We need the following trigonometric identity.

**4.1 Lemma.**

$$2 \sum_{r=0}^n \cos(r\theta) = \frac{\sin((n + \frac{1}{2})\theta)}{\sin(\frac{1}{2}\theta)} + 1.$$

*Proof.* If  $q := e^{i\theta}$  then

$$\begin{aligned} 2 \sum_{r=0}^n \cos(r\theta) &= \sum_{r=0}^n (q^r + q^{-r}) \\ &= \frac{q^{n+1} - 1}{q - 1} + \frac{q^{-n-1} - 1}{q^{-1} - 1} \\ &= \frac{q^{n+1} - 1}{q - 1} + \frac{q^{-n} - q}{1 - q} \\ &= \frac{q^{n+1} - q^{-n}}{q - 1} + 1 \\ &= \frac{q^{n+1/2} - q^{-1/2-n}}{q^{1/2} - q^{-1/2}} + 1 \\ &= \frac{\sin((n + \frac{1}{2})\theta)}{\sin(\frac{1}{2}\theta)} + 1. \end{aligned} \quad \square$$

We will also use the following explicit expression for the idempotents in the spectral decomposition of  $A(P_n)$ . This result is standard, but we offer a sketch of the proof.

**4.2 Lemma.** *The idempotents  $E_1, \dots, E_n$  in the spectral decomposition of  $P_n$  are given by*

$$(E_r)_{j,k} = \frac{2}{n+1} \sin\left(\frac{jr\pi}{n+1}\right) \sin\left(\frac{kr\pi}{n+1}\right).$$

*Proof.* If  $A = A(P_n)$  and  $e_n$  is the  $n$  vector in the standard basis of  $\mathbb{R}^n$ , then

$$A \begin{pmatrix} \sin(\beta) \\ \sin(2\beta) \\ \vdots \\ \sin(n\beta) \end{pmatrix} = \begin{pmatrix} \sin(2\beta) \\ \sin(\beta) + \sin(3\beta) \\ \vdots \\ \sin((n-1)\beta) \end{pmatrix} = 2 \cos(\beta) \begin{pmatrix} \sin(\beta) \\ \sin(2\beta) \\ \vdots \\ \sin(n\beta) \end{pmatrix} - \sin((n+1)\beta) e_n$$

So if  $\sin((n+1)\beta) = 0$  then

$$z(\beta) := \begin{pmatrix} \sin(\beta) \\ \sin(2\beta) \\ \vdots \\ \sin(n\beta) \end{pmatrix}$$

is an eigenvector for  $A$  with eigenvalue  $2 \cos(\beta)$ . Letting  $\beta$  vary over the values

$$\frac{2\pi r}{n+1}, \quad r = 1, \dots, n$$

we obtain  $n$  distinct eigenvalues. Therefore each eigenvalue of  $P_n$  is simple and the projection onto the eigenspace spanned by  $z(\beta)$  is

$$\frac{1}{z(\beta)^T z(\beta)} z(\beta) z(\beta)^T.$$

We can compute the value of the inner product  $z(\beta)^T z(\beta)$  using Lemma 4.1, and this yields the stated expression for  $E_r$ .  $\square$

**4.3 Lemma.** *If  $E_1, \dots, E_n$  are the idempotents for  $P_n$ , then the average mixing matrix of  $P_n$  is*

$$\sum_r E_r \circ E_r = \frac{1}{2n+2} (2J + I + T).$$



*Proof.* We use Lemma 4.2:

$$(E_r \circ E_r)_{j,k} = \frac{4}{(n+1)^2} \sin^2\left(\frac{jr\pi}{n+1}\right) \sin^2\left(\frac{kr\pi}{n+1}\right)$$

which implies that

$$\frac{(n+1)^2}{4} (E_r \circ E_r)_{j,k} = \frac{1}{4} \left(1 - \cos\left(\frac{2jr\pi}{n+1}\right)\right) \left(1 - \cos\left(\frac{2kr\pi}{n+1}\right)\right).$$

Now

$$\begin{aligned} & \left(1 - \cos\left(\frac{2jr\pi}{n+1}\right)\right) \left(1 - \cos\left(\frac{2kr\pi}{n+1}\right)\right) = \\ & 1 - \cos\left(\frac{2jr\pi}{n+1}\right) - \cos\left(\frac{2kr\pi}{n+1}\right) + \frac{1}{2} \cos\left(\frac{2(j+k)r\pi}{n+1}\right) + \frac{1}{2} \cos\left(\frac{2(j-k)r\pi}{n+1}\right) \end{aligned}$$

We need to sum each of the five terms on the right from 1 to  $n$ . From Lemma 4.1 it follows that

$$\sum_{r=1}^n \cos\left(\frac{2\ell r\pi}{n+1}\right) = \frac{1}{2} \left(-1 + \frac{\sin\left(\frac{(2n+1)\ell\pi}{n+1}\right)}{\sin\left(\frac{\ell\pi}{n+1}\right)}\right) = \frac{1}{2} \left(-1 + \frac{\sin\left(2\ell\pi - \frac{\ell\pi}{n+1}\right)}{\sin\left(\frac{\ell\pi}{n+1}\right)}\right) = -1.$$

Consequently

$$\sum_{r=1}^n (n+1)^2 (E_r \circ E_r)_{j,k} = \begin{cases} 3(n+1)/2, & j = k; \\ 3(n+1)/2, & j + k = n+1 \\ n+1, & \text{otherwise} \end{cases}$$

and this completes the proof.  $\square$

## 5 Path Laplacians

Let  $\Delta$  denote the diagonal matrix with  $i$ -th diagonal entry equal to the valency of the  $i$ -th vertex of  $X$ . Then the Laplacian of  $X$  is  $\Delta - A$ . Let  $D$  be the  $n \times (n-1)$  matrix with

$$D_{i,i} = 1, \quad D_{i,i-1} = -1$$

and all other entries zero. Then  $D$  is the incidence matrix of an orientation of  $P_n$  and

$$DD^T = \Delta - A(P_n), \quad D^T D = 2I - A(P_{n-1}).$$

If  $\theta_1, \dots, \theta_{n-1}$  are the eigenvalues of  $P_{n-1}$ , this shows that the non-zero eigenvalues of  $\Delta - A(P_n)$  are the numbers  $2 - \theta_r$  for  $r = 1, \dots, n-1$ . We can also use this to determine the idempotents in the spectral decomposition of  $\Delta - A(P_n)$ . The lemma follows.  $\square$

**5.1 Lemma.** *If  $E_1, \dots, E_{n-1}$  are the idempotents in the spectral decomposition of  $P_{n-1}$ , then the idempotents of  $\Delta - A(P_n)$  are  $n^{-1}J$  and*

$$\frac{1}{2 - \theta_r} DE_r D^T, \dots, r = 1, \dots, n-1.$$

*Proof.* Since

$$DE_r D^T DE_s D^T = DE_r (2I - A(P_{n-1})E_s D^T)$$

and since  $E_r E_s = 0$  if  $r \neq s$  and  $(2I - A(P_{n-1})E_s = (2 - \theta_s)E_s$ , it follows that

$$DE_r D^T DE_s D^T = \delta_{r,s} (2 - \theta_r) DE_r D^T.$$

Therefore  $(2 - \theta_r)^{-1} DE_r D^T$  is an idempotent. Next

$$(\Delta - A(P_n)) DE_r D^T = DD^T DE_r D^T = D(2I - A(P_{n-1}))E_r D^T = (2 - \theta_r) DE_r D^T$$

and therefore  $(2 - \theta_r)^{-1} DE_r D^T$  represents orthogonal projection onto an eigenspace of  $A(P_n)$ . The lemma follows.  $\square$

**5.2 Lemma.** *If  $E_1, \dots, E_{n-1}$  are the idempotents in the spectral decomposition of  $P_{n-1}$ , then*

$$(2 - \theta_r)^{-1} (DE_r D^T)_{j,k} = \frac{2}{n} \cos\left(\frac{(2j-1)r\pi}{2n}\right) \cos\left(\frac{(2k-1)r\pi}{2n}\right), \quad 1 \leq j, k \leq n.$$

*Proof.* From Lemma 4.2, we have

$$(E_r)_{j,k} = \frac{2}{n} \sin\left(\frac{jr\pi}{n}\right) \sin\left(\frac{kr\pi}{n}\right), \quad 1 \leq j, k \leq n-1.$$

Let  $\alpha = r\pi/n$  and let  $\sigma$  denote the column vector of length  $n-1$  where  $\sigma_j = \sin(j\alpha)$ . Then

$$DE_r D^T = \frac{2}{n} D\sigma(D\sigma)^T$$

and

$$D\sigma = \begin{pmatrix} \sin(\alpha) \\ \sin(2\alpha) - \sin(\alpha) \\ \vdots \\ \sin((n-1)\alpha) - \sin((n-2)\alpha) \\ -\sin((n-1)\alpha) \end{pmatrix} = 2\sin(\alpha/2) \begin{pmatrix} \cos(\alpha/2) \\ \cos(3\alpha/2) \\ \vdots \\ \cos((2n-3)\alpha/2) \\ \cos((2n-1)\alpha/2) \end{pmatrix},$$

where in computing the last entry we have used the fact that  $n\alpha = r\pi$ , whence  $\sin(n\alpha) = 0$  and

$$-\sin(n-1)\alpha = \sin(n\alpha) - \sin(n-1)\alpha.$$

Finally for  $P_{n-1}$  we have

$$2 - \theta_r = 2 - 2\cos\left(\frac{r\pi}{n}\right) = 4\sin^2\left(\frac{r\pi}{2n}\right)$$

**5.3 Theorem.** *The average mixing matrix for the continuous quantum walk using the Laplacian matrix of the path  $P_n$  is*

$$\frac{1}{n^2} \left( (n-1)J + \frac{n}{2}(I + T) \right).$$

*Proof.* Set

$$F_r = (2 - \theta_r)^{-1} D E_r D^T.$$

Then

$$\begin{aligned} (F_r^{\circ 2})_{j,k} &= \frac{4}{n^2} \cos^2\left(\frac{(2j-1)r\pi}{2n}\right) \cos^2\left(\frac{(2k-1)r\pi}{2n}\right) \\ &= \frac{1}{n^2} \left( 1 + \cos\left(\frac{(2j-1)r\pi}{n}\right) \right) \left( 1 + \cos\left(\frac{(2k-1)r\pi}{n}\right) \right) \end{aligned}$$

and

$$\begin{aligned} &\left( 1 + \cos\left(\frac{(2j-1)r\pi}{n}\right) \right) \left( 1 + \cos\left(\frac{(2k-1)r\pi}{n}\right) \right) \\ &= 1 + \cos\left(\frac{(2j-1)r\pi}{n}\right) + \cos\left(\frac{(2k-1)r\pi}{n}\right) \\ &\quad + \frac{1}{2} \cos\left(\frac{(2j+2k-2)r\pi}{n}\right) + \frac{1}{2} \cos\left(\frac{(2j-2k)r\pi}{n}\right). \end{aligned}$$

From Lemma 4.1 we have

$$\begin{aligned}
2 \sum_{r=1}^{n-1} \cos\left(\frac{r\ell\pi}{n}\right) &= -1 + \frac{\sin\left((n - \frac{1}{2})\frac{\ell\pi}{n}\right)}{\sin\left(\frac{\ell\pi}{2n}\right)} \\
&= -1 + \frac{\sin\left(\ell\pi - \frac{\ell\pi}{2n}\right)}{\sin\left(\frac{\ell\pi}{2n}\right)} \\
&= -1 + \frac{-\cos(\ell\pi) \sin\left(\frac{\ell\pi}{2n}\right)}{\sin\left(\frac{\ell\pi}{2n}\right)} \\
&= -((-1)^\ell + 1).
\end{aligned}$$

It is now easy to derive the stated formula for the average mixing matrix.  $\square$

We note that  $2I - L(P_n)$  can be viewed as the adjacency matrix of a path on  $n$  vertices with a loop of weight one on each end-vertex. Examples show that if we add loops with weight other than 0 or 1, the average mixing matrix is not a linear combination of  $I$ ,  $J$  and  $T$ . Thus if we add loops of weight 2 to the end-vertices of  $P_6$ , the average mixing matrix is:

$$\frac{1}{2 * 9 * 107} \begin{pmatrix} 599 & 218 & 146 & 146 & 218 & 599 \\ 218 & 455 & 290 & 290 & 455 & 218 \\ 146 & 290 & 527 & 527 & 290 & 146 \\ 146 & 290 & 527 & 527 & 290 & 146 \\ 218 & 455 & 290 & 290 & 455 & 218 \\ 599 & 218 & 146 & 146 & 218 & 599 \end{pmatrix}.$$

(Here the discriminant of the characteristic polynomial is  $2^6 3^5 107$ .)

## 6 Cycles

We determine the average mixing matrices for cycles.

Let  $P$  be the permutation matrix corresponding to a cycle of length  $n$  and let  $\zeta$  be a primitive  $n$ -th root of unity. Define matrices  $F_0, \dots, F_{n-1}$  by

$$(F_r)_{i,j} = \frac{1}{n} \zeta^{r(i-j)}.$$

(Thus the rows and columns of these matrices are indexed by  $\{0, \dots, n-1\}$ .) Then  $P$  is a normal matrix and has the spectral decomposition

$$P = \sum_{r=0}^{n-1} \zeta^r F_r.$$

We also note that

$$F_r \circ F_s = \frac{1}{n} F_{r+s}$$

where the subscripts are viewed as elements of  $\mathbb{Z}_n$ . The adjacency matrix of the cycle on  $n$  vertices is  $P + P^T$ . Define  $E_0$  to be  $F_0$  and, if  $0 < r < n/2$ , we set

$$E_r = F_r + F_{n-r}.$$

Further  $E_0 := F_0$  and, if  $n$  is even then  $E_{n/2} := F_{n/2}$ . Then if  $n$  is odd,

$$E_0, \dots, E_{(n-1)/2}$$

are the idempotents in the spectral decomposition of  $A(C_n)$  and the corresponding eigenvalues are

$$\theta_r = \zeta^r + \zeta^{-r}, \quad r = 0, \dots, \frac{n-1}{2};$$

if  $n$  is even we have the additional idempotent  $E_{n/2}$  with eigenvalue  $\zeta^{n/2} = -1$ .

**6.1 Lemma.** *If  $n$  is odd then the average mixing matrix of the cycle  $C_n$  is*

$$\frac{n-1}{n^2} J + \frac{1}{n} I,$$

*if  $n$  is even it is*

$$\frac{n-2}{n^2} J + \frac{1}{n} (I + P^{n/2}).$$

*Proof.* Assume first that  $n = 2m + 1$ . Then the average mixing matrix is

$$\begin{aligned} \sum_{r=0}^m E_r^{\circ 2} &= F_0^{\circ 2} + \sum_{r=1}^m (F_r + F_{-r})^{\circ 2} \\ &= \frac{1}{n} F_0 + \frac{1}{n} \sum_{r=1}^m (F_{2r} + F_{-2r} + 2F_0) \\ &= F_0 + \frac{1}{n} \sum_{r=1}^{n-1} F_r \\ &= \frac{1}{n} I + \frac{n-1}{n} F_0. \end{aligned}$$

Now suppose  $n = 2m$ . Then the average mixing matrix is

$$\begin{aligned}
E_m^{\circ 2} + \sum_{r=0}^{m-1} E_r^{\circ 2} &= F_0^{\circ 2} + F_m^{\circ 2} + \sum_{r=1}^{m-1} (F_r + F_{-r})^{\circ 2} \\
&= \frac{1}{n} F_0 + \frac{1}{n} F_0 + \frac{1}{n} \sum_{r=1}^{m-1} (F_{2r} + F_{-2r} + 2F_0) \\
&= F_0 + \frac{1}{n} \sum_{r=1}^{m-1} (F_{2r} + F_{-2r}) \\
&= \frac{n-2}{n} F_0 + \frac{2}{n} \sum_{r=0}^{m-1} F_{2r}.
\end{aligned}$$

Since

$$P^m F_s = (\zeta^m)^s F_s = (-1)^s F_s$$

we see that  $P^m$  has spectral decomposition

$$P^m = \sum_{s=0}^{n-1} (-1)^s F_s$$

and consequently

$$\frac{1}{2}(I + P^m) = \sum_{r=0}^{m-1} F_{2r}.$$

Our stated formula for the average mixing matrix follows.  $\square$

In general the average mixing matrix for a circulant can be more complex in structure than the average mixing matrix of a cycle. We will see in the next section that graphs in pseudocyclic schemes provide the right generalization of cycles or, at least, of odd cycles.

It is easy for different circulants of order  $n$  to have the same spectral idempotents, any two such circulants necessarily have the same average mixing matrix.

## 7 Pseudocyclic Schemes

An association scheme  $\mathcal{A}$  with  $d$  classes on  $v$  vertices is a set of 01-matrices  $A_0, \dots, A_d$  such that

- (a)  $A_0 = I$  and  $\sum_i A_i = J$ .

- (b) For each  $i$  we have  $A_i^T \in \mathcal{A}$ .
- (c)  $A_i A_j = A_j A_i$ .
- (d) For all  $i$  and  $j$  the product  $A_i A_j$  lies in the real span of  $\mathcal{A}$ .

Convenient references are [2, 3]. We often view the matrices  $A_i$  as the adjacency matrices of directed graphs on  $v$  vertices, we call these the *graphs* of the scheme and note that the axioms are often stated in terms of the graphs rather than their adjacency matrices. An association scheme is *symmetric* if each matrix in it is symmetric. These axioms imply that the span of  $\mathcal{A}$  is a commutative matrix algebra that is closed under the Schur product. It is called the *Bose-Mesner algebra* of the scheme. The matrices in  $\mathcal{A}$  form a basis consisting of Schur idempotents. There is also a basis of matrix idempotents  $E_0, \dots, E_d$ , which satisfy

- (a)  $E_0 = v^{-1}J$  and  $\sum E_j = I$ .
- (b) For each  $j$  there is an index  $j'$  such that  $\bar{E}_j = E_{j'}$ .
- (c) For all  $i$  and  $j$  the Schur product  $E_i \circ E_j$  lies in the Bose-Mesner algebra.

The matrix idempotents can be viewed as providing (an analog of) the spectral decomposition.

Since the matrices  $A_i$  commute it follows that  $A_i$  and  $J$  commute and hence there are constants  $v_i$  such that  $A_i J = v_i J$ , these are the *valencies* of the scheme. The column space of  $E_j$  is an eigenspace for all matrices in the Bose-Mesner algebra, its dimension is denoted by  $m_j$  and it is referred to as a *multiplicity* of the scheme. Note that  $v_0 = m_0 = 1$ . A scheme is *pseudocyclic* if  $m_1, \dots, m_d$  are equal (in which case their common value is  $(v-1)/d$ ). If a scheme is pseudocyclic then  $v_1, \dots, v_d$  are necessarily all equal to  $(v-1)/d$ . For details see Brouwer, Cohen and Neumaier[2, §2.2B].

We note one class of examples, the *cyclotomic schemes*. Assume  $q$  is a prime power and  $d$  divides  $q-1$ . Let  $\mathbb{F}$  be the finite field of order  $q$  and let  $S$  be the subgroup of the multiplicative group of  $\mathbb{F}$  generated by the non-zero  $d$ -th powers. Thus  $|S| = (q-1)/d$ . Let  $S_1, \dots, S_d$  denote the cosets of  $S$  in  $\mathbb{F}^*$ , with  $S_1 = S$ . Now we define the matrices of an association scheme with  $d$  classes and with vertex set  $\mathbb{F}$  by setting  $A_0 = I$  and

$$(A_i)_{x,y} = 1, \quad (i = 1, \dots, d)$$

if and only if  $y - x$  is in  $S_i$ . These matrices form the cyclotomic scheme with  $d$  classes on  $\mathbb{F}$ . It is symmetric if and only if  $-1 \in S$ . The directed graphs  $X_1, \dots, X_d$  such that  $A_i = A(X_i)$  are all isomorphic. The most well known case is when  $d = 2$  and  $q \cong 1$  modulo four, in which case the two graphs we have constructed are the *Paley graphs*.

We note that there are pseudocyclic schemes which are not cyclotomic, and that there are pseudocyclic schemes with two classes where the two graphs are asymmetric, that is, their only automorphism is the identity.

## 8 Average Mixing on Pseudocyclic Graphs

**8.1 Theorem.** *Suppose  $X$  is a graph in a  $d$ -class pseudocyclic scheme on  $n$  vertices consisting of graphs of valency  $m = (n - 1)/d$ . Then the average mixing matrix of  $X$  is*

$$\frac{n - m + 1}{n^2}J + \frac{m - 1}{n}I.$$

*Proof.* Koppinen [7] proved that for an association scheme with  $d$  classes we have

$$\sum_{i=0}^d \frac{1}{nv_i} A_i \otimes A_i^T = \sum_{j=0}^d \frac{1}{m_j} E_j \otimes E_j.$$

If the scheme is symmetric then  $A_i \circ A_i = A_i$  and, since  $M \circ N$  is a submatrix of  $M \otimes N$ , Koppinen's identity yields that

$$\sum_{i=0}^d \frac{1}{nv_i} A_i = \sum_{j=0}^d \frac{1}{m_j} E_j \circ E_j.$$

For any scheme, we have  $m_0 = v_0 = 1$  and for a pseudocyclic scheme

$$m_i = v_i = \frac{n - 1}{d}, \quad i = 1, \dots, d.$$

As  $\sum_i A_i = J$  and  $\sum_j E_j = I$ , if  $m = (n - 1)/d$  we find that

$$\frac{1}{n} \left( I + \frac{1}{m} (J - I) \right) = \frac{1}{n^2} J + \frac{1}{m} \sum_{j=1}^d E_j^{\circ 2}$$

and hence

$$\frac{1}{m} \sum_{j=1}^d E_j^{\circ 2} = \left( \frac{1}{nm} - \frac{1}{n^2} \right) J + \frac{m - 1}{nm} I = \frac{n^2 - nm}{n^3 m} J + \frac{m - 1}{nm} I. \quad \square$$



A graph in a pseudocyclic scheme with two classes is known as a *conference graph*, and there are examples whose automorphism group is trivial.

## 9 Cospectral Vertices

If  $u \in V(X)$  then  $(A^k)_{u,u}$  is equal to the number of closed walks on  $X$  of length  $k$  that start (and finish) at  $u$ . The following result summarizes some standard facts. (The equivalence of (a) and (c) follows from Equation (1) on page 52 of [3] and (a) and (b) from Equation (2) on page 9 of the same source.)

**9.1 Theorem.** *Let  $X$  be a graph with vertices  $u$  and  $v$ , and let  $E_1, \dots, E_m$  be the idempotents in the spectral decomposition of  $A(X)$ . Then the following are equivalent:*

- (a)  $(A^k)_{u,u} = (A^k)_{v,v}$  for all  $k \geq 0$ .
- (b)  $\|E_r e_u\|^2 = \|E_r e_v\|^2$ .
- (c) *The graphs  $X \setminus u$  and  $X \setminus v$  are cospectral.* □

Note that

$$\|E_r e_u\|^2 = e_u^T E_r^T E_r e_u = e_u^T E_r^2 e_u = e_u^T E_r e_u = (E_r)_{u,u}.$$

We will say that vertices  $u$  and  $v$  of  $X$  are *cospectral* if any of the conditions in this theorem hold.

We recall that the graph  $X$  admits *perfect state transfer* from  $u$  to  $v$  at time  $\tau$  if there is a scalar  $\gamma$  such that

$$H_X(\tau) e_u = \gamma e_v$$

where  $|\gamma| = 1$  since  $\|e_u\| = \|H_X(\tau) e_u\|$ . As  $H_X(t)$  is a polynomial in  $A$ , we have

$$E_r H_X(t) = H_X(t) E_r = \exp(i\theta_r t) E_r$$

and therefore

$$\gamma E_r e_v = H_X(\tau) E_r e_u = \exp(i\theta_r \tau) E_r e_v.$$

Since  $E_r e_v$  and  $E_r e_u$  are real vectors and since  $|\gamma| = |\exp(i\theta_r \tau)| = 1$ , we conclude that

$$E_r e_u = \pm E_r e_v.$$

(This fact is well known and we include the proof for convenience only.)

Clearly if  $E_r e_u = \pm E_r e_v$  then

$$\|E_r e_u\|^2 = \|E_r e_v\|^2$$

and so  $u$  and  $v$  are cospectral. We will say that  $u$  and  $v$  are *strongly cospectral* if  $E_r e_u = \pm E_r e_v$ .

**9.2 Lemma.** *If  $u$  and  $v$  are vertices in  $X$  and the eigenvalues of  $X$  are simple, then  $u$  and  $v$  are strongly cospectral if and only if they are cospectral.*

*Proof.* We only need to consider the case where  $u$  and  $v$  are cospectral. The vectors  $E_r e_u$  and  $E_r e_v$  are both eigenvectors of  $X$  with eigenvalue  $\theta_r$ . Since  $\theta_r$  is simple this means that  $E_r e_v$  is a scalar multiple of  $E_r e_u$ . Since these two vectors have the same length, the lemma follows.  $\square$

**9.3 Theorem.** *Let  $\widehat{M}_X$  be the average mixing matrix of the graph  $X$ . Then vertices  $u$  and  $v$  are strongly cospectral if and only if  $\widehat{M}_X(e_u - e_v) = 0$ .*

*Proof.* Suppose  $N \succcurlyeq 0$  and  $N(e_1 - e_2) = 0$ . We may assume that the leading  $2 \times 2$  submatrix of  $N$  is

$$\begin{pmatrix} a & b \\ b & d \end{pmatrix}$$

and therefore

$$0 = (e_1 - e_2)^T N(e_1 - e_2) = a + d - 2b.$$

Hence  $b = (a + d)/2$ . Since  $N \succcurlyeq 0$  we have  $ad - b^2 \geq 0$  and thus

$$0 \leq 4ad - 4b^2 = 4ad - (a + d)^2 = -(a - d)^2,$$

whence  $a = d = b$ .

If  $\widehat{M}_X(e_u - e_v) = 0$  then

$$0 = (e_u - e_v)^T \widehat{M}_X(e_u - e_v) = \sum_r (e_u - e_v)^T E_r^{\circ 2} (e_u - e_v)$$

and as each summand  $E_r^{\circ 2}$  in  $\widehat{M}_X$  is positive semidefinite, we have

$$E_r^{\circ 2}(e_u - e_v) = 0$$

for all  $r$ . Therefore, for all  $r$ ,

$$((E_r)_{u,u})^2 = ((E_r)_{u,v})^2 = ((E_r)_{v,v})^2$$

Since

$$(E_r)_{u,v} = \langle E_r e_u, E_r e_v \rangle$$

it follows by Cauchy-Schwarz that  $E_r e_u = \pm E_r e_v$ .  $\square$

A graph is *walk regular* if all its vertices are cospectral. There are many classes of examples, and it is not necessary that such graphs be vertex transitive. We note the following though:

**9.4 Lemma.** *If all vertices in  $X$  are strongly cospectral, then  $X$  is  $K_1$  or  $K_2$ .*

*Proof.* If all vertices are strongly cospectral, then all rows of  $\widehat{M}_X$  are equal, and therefore it is a scalar multiple of  $J$ . By [4, Lemma 16.2] this implies that  $|V(X)| \leq 2$ .  $\square$

One consequence of the results here is that, if the rows of the average mixing matrix of  $X$  are distinct, there is no perfect state transfer on  $X$ . Kay [5, Section D] has shown that if we have perfect state transfer in  $X$  from  $u$  to  $v$  and from  $u$  to  $w$ , then  $v = w$ .

## 10 Discrete Walks

If  $U$  is a unitary matrix then its powers describe a *discrete quantum walk*. The corresponding average mixing matrix is

$$\lim_{N \rightarrow \infty} \frac{1}{N} \sum_{n=0}^{N-1} U^n \circ U^{-n}.$$

Since unitary matrices are normal, they have a spectral decomposition which we can write as

$$U = \sum_r e^{i\theta_r} E_r$$

where  $\theta_r$  is real and  $E_r$  Hermitian for all  $r$ . The unitary matrices considered in quantum computing are constructed from an underlying regular graph.

**10.1 Theorem.** *If  $E_1, \dots, E_m$  are the idempotents in the spectral decomposition of the unitary matrix  $U$ , the average mixing matrix  $\widehat{U}$  of  $U$  is  $\sum_r E_r^{\circ 2}$ . If  $U$  is rational then  $\widehat{U}$  is rational.*

*Proof.* We have

$$U^n \circ U^{-n} = \sum_r E_r^{\circ 2} + \sum_{r \neq s} e^{ni(\theta_r - \theta_s)} E_r \circ E_s.$$

Therefore

$$\frac{1}{N} \sum_{n=0}^{N-1} U^n \circ U^{-n} = \sum_r E_r^{\circ 2} + \frac{1}{N} \left( \sum_{n=0}^{N-1} e^{ni(\theta_r - \theta_s)} \right) E_r \circ E_s$$

and since

$$\sum_{n=0}^{N-1} e^{ni(\theta_r - \theta_s)} = \frac{e^{ni(\theta_r - \theta_s)} - 1}{e^{i(\theta_r - \theta_s)} - 1}$$

The right side is bounded in absolute value by

$$\frac{2}{|e^{i(\theta_r - \theta_s)} - 1|}$$

which is independent of  $N$ . Hence

$$\frac{1}{N} \sum_{n=0}^{N-1} U^n \circ U^{-n} \rightarrow \sum_r E_r^{\circ 2}$$

as  $N$  tends to infinity. □

Since

$$I - U^n \circ U^{-n} = \sum_{r \neq s} (1 - e^{ni(\theta_r - \theta_s)}) E_r \circ E_s = 2 \sum_{r \neq s} (1 - \cos(n(\theta_r - \theta_s))) E_r \circ E_s,$$

we see that  $I - U^n \circ U^{-n}$  is positive semidefinite and hence  $I - \widehat{U}$  is positive semidefinite.

If  $U$  is based on a regular graph then  $\widehat{U}$  is rational.

## 11 Questions

We list three questions raised by our work.

1. Is it true that if  $D$  is the discriminant of the minimal polynomial of  $X$ , then  $D\widehat{M}_X$  is an integer matrix?
2. Is there a useful algorithm for computing  $\widehat{M}_X$  that works over the rationals?
3. Which graph have the property that their average mixing matrix is a linear combination of  $I$  and  $J$ ? (Jamie Smith, in unpublished work, has found a strongly regular graph with this property that is not pseudocyclic.)

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## References

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